AEDC-TR-85-52
ESL-TR-83-54

Space Shuttle HCl Gas Detection

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Sverdrup Technology, Inc.

May 1987

Final Report for Period April 15, 1984 — May 15, 1985

DOC NUM
UNC29747-PDC
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ARNOLD ENGINEERING DEVELOPMENT CENTER
ARNOLD AIR FORCE STATION, TENNESSEE
AIR FORCE SYSTEMS COMMAND
UNITED STATES AIR FORCE

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This report has been reviewed and approved.

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Deputy for Operations

Approved for publication:

FOR THE COMMANDER

MARION L. LASTER
Director of Technology
Deputy for Operations

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b. RESTRICTIVE MARKINGS

2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT SEE REVERSE OF THIS PAGE
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	

4. PERFORMING ORGANIZATION REPORT NUMBER(S) AEDC-TR-85-52	5. MONITORING ORGANIZATION REPORT NUMBER(S)

6a. NAME OF PERFORMING ORGANIZATION Arnold Engineering Development Center	6b. OFFICE SYMBOL (If applicable) DOT	7a. NAME OF MONITORING ORGANIZATION

6c. ADDRESS (City, State and ZIP Code) Air Force Systems Command Arnold Air Force Station, TN 37389-5000	7b. ADDRESS (City, State and ZIP Code)

8a. NAME OF FUNDING/SPONSORING ORGANIZATION Air Force Engineering Services Center	8b. OFFICE SYMBOL (If applicable) RDVS	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER

8c. ADDRESS (City, State and ZIP Code) Tyndall Air Force Base, Florida 32403	10. SOURCE OF FUNDING NOS			
	PROGRAM ELEMENT NO	PROJECT NO	TASK NO	WORK UNIT NO
11. TITLE (Include Security Classification) SEE REVERSE OF THIS PAGE	921A67			

12. PERSONAL AUTHOR(S)   Scott, M. G. and Pender, C. W., Jr., Sverdrup Technology, Inc., AEDC Group

13a. TYPE OF REPORT Final	13b. TIME COVERED FROM 4/15/84 TO 5/15/85	14. DATE OF REPORT (Yr., Mo., Day) May 1987	15. PAGE COUNT 30

16. SUPPLEMENTARY NOTATION   Available in Defense Technical Information Center (DTIC).

17	COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB GR	HCl concentrations Space Shuttle solid-propellant
21	02		Fourier transform data acquisition rocket boosters
01	03		spectrometer combustion byproducts

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Hydrogen chloride (HCl) gas is one of the byproducts produced by the Space Shuttle solid-propellant rocket boosters. This report describes a nonobtrusive absorption technique to measure concentrations of gaseous HCl for four days following Shuttle launches 41D and 51A at Kennedy Space Center (KSC). The peak concentrations measured near ground level about 400 m from the launch structure were found to be less than 10 ppm averaged over a 500-m path after both launches.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☒ DTIC USERS ☐	21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED

22a. NAME OF RESPONSIBLE INDIVIDUAL W. O. Cole	22b. TELEPHONE NUMBER (Include Area Code) (615)454-7813	22c. OFFICE SYMBOL DOS

DD FORM 1473, 83 APR   EDITION OF 1 JAN 73 IS OBSOLETE

3. DISTRIBUTION/AVAILABILITY OF REPORT

Approved for public release; distribution is unlimited.

11. TITLE

Space Shuttle HCl Gas Detection

PREFACE

The work reported herein was conducted by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC), at the request of Air Force Engineering Services Center (AFESC/RDVS), Tyndall Air Force Base, Florida, and the Atmospheric Effects Branch, Marshall Space Flight Center, NASA H-73999B. The reported measurements were conducted and results obtained by Sverdrup Technology, Inc., AEDC Group, operating contractor for the propulsion test facilities at the AEDC, AFSC, Arnold Air Force Station, Tennessee, under Project Number DB07EW. The Air Force Project Managers were Captain Frank Tanji and Captain Bradley Biehn, AEDC/DOTR. The data analysis was completed on May 15, 1985, and the manuscript was submitted for publication on July 1, 1985.

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1.0 INTRODUCTION

Large amounts of gaseous hydrogen chloride (HCl) are one of the combustion by-products generated during the launch of the Space Transportation System (Shuttle) by the Shuttle's solid-propellant rocket boosters (SRB's). Significant quantities of HCl are present in the plume cloud that lingers near the launch structure. The HCl gas remains entrained in the atmosphere near the launch facility, is dispersed by wind, and is deposited on surfaces, such as grass or ground. (See Ref. 1 for deposition mechanisms.) The HCl gas that remains in the vicinity of the launch structure, from either initial release or secondary ground release, is important because it corrodes metals and electronic equipment and because it is a health hazard. The problem is currently restricted to the Kennedy Space Center (KSC) launch area but will also be present at Vandenberg when the Shuttle Western Test Range launch facility is activated. The problem may be exacerbated at Vandenberg because of differences in the launch mount, sound-suppression water systems, and the proximity of the launch facilities.

The objective of this project was to develop and apply a nonobtrusive absorption technique employing a Fourier Transform Spectrometer (FTS) to monitor the concentration of gaseous HCl present near the KSC launch pad for several days after a Shuttle launch. Because of safety considerations and the requirement to collect data immediately after a launch, the measurement technique was automated to permit untended operation. The technique was applied for launches 41D and 51A, Pad 39A (Fig. 1), which occurred on August 30, 1984 and November 8, 1984, respectively, at KSC.

To accomplish the objective, a technique based on the absorption of infrared (IR) radiation by the diatomic HCl molecules was developed. The characteristic HCl lines are attributable to absorption of radiation associated with vibrational and rotational transitions within the HCl molecule. A simple model (Ref. 2) to describe this absorption process is a molecule in which the individual atoms, held together by chemical bonds, are in vibratory motion along these bonds, while the entire molecule is rotating. The HCl is in a state of vibratory motion brought about by the alternate stretching and contracting of the chemical bond as the hydrogen and chlorine atoms move away and toward each other, respectively. This vibratory motion is superimposed on a rotation of the molecule about an axis perpendicular to the chemical bond. When IR radiation of the proper frequency (i.e. energy) impinges on the molecule and is absorbed, the vibration and/or rotation states are changed. These changes must satisfy certain selection rules that give rise to discrete absorption lines. These lines are labeled according to their frequency. The lines with frequencies greater than that of the band center are said to be in the R branch, whereas those with frequencies less than that of the band center are in the P branch (Fig. 2). The individual lines making up the P and R branches are identified as P(1), P(2), etc. as the frequency of the lines moves away from the band center.

2.0 TECHNIQUE

A nonobtrusive IR absorption technique was used for monitoring gaseous HCl concentrations over long paths near the Shuttle launch pad (Fig. 1). The technique involved use of an IR spectrometer located approximately 500 m from an IR source. An IR spectrum was acquired at regular intervals (20 min for 41D, 10 min for 51A) for several days following the Shuttle launches. The spectra were then inspected to find the magnitude of absorption because of the presence of gaseous HCl. The concentration of HCl was then calculated using the absorption coefficient measured in the laboratory. The spectral line used to determine the amount of absorption is in the band centered at 2,886 cm^{-1}. This technique is not dependent on absolute magnitudes of the spectra; therefore, the intensity of the source is not relevant to the measurement, and only relative intensities will be presented in this report.

Naturally occurring HCl contains two isotopes of chlorine. They are ^{35}Cl and ^{37}Cl, in the ratio of 3 to 1, respectively. The IR absorption lines of H^{35}Cl and H^{37}Cl are separate, but very close. A spectrum of these isotopic species is shown in Fig. 2b.

The absorption attributable to HCl gas is well understood and documented. The HCl absorption lines are described by (Ref. 3)

$$I(\lambda) = I_o(\lambda) \exp \left\{ -SP\gamma_o L/[(\lambda - \lambda_o)^2 + \gamma_o^2]\pi \right\}$$

where

I$_o$ (λ) is the intensity of the incident radiation

I (λ) is the intensity of the transmitted radiation

S is the line strength of the absorption line (cm^{-2} atm^{-1})

P is the partial pressure of the absorbing species (atm)

γ_o is the pressure-broadened half-width at half-maximum of the HCl line (cm^{-1})

λ_o is the line center of the absorption line (cm^{-1})

L is path length

Figure 3 shows the P(1) lines calculated using parameters contained in Ref. 4. The figure shows the theoretical absorption assuming 6 ppm HCl over a 500-m path. Because of limited resolution and the apodization function, the Fourier transform spectrometer (FTS) that produced the actual spectra influences the spectra shape. The convolution of the instrument line shape (ILS), using 0.5-cm^{-1} resolution and a triangular apodization function, produces the P(1) line shown in Fig. 3b. As can be seen by comparing Figs. 3a and b, the ILS shortens

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and broadens the spectral lines. (Note: The scales of these plots are not the same.) The effect is detrimental in that the resultant spectrum is not an accurate portrayal of the true line shape. However, it is still possible to use the resultant spectra since the effect can be calibrated. The calibration will be discussed later in this report.

A complicating factor was the presence of additional absorption lines in the spectra obtained in the field. The effect of neighboring absorption lines is to give the impression of a greater amount of gaseous HCl. The spectral region of interest included absorption lines attributable to other molecules present in the atmosphere such as H_2O and, Hydrogen Deuterium Oxide (HDO) (Ref. 5). Therefore, the spectra were obtained at 0.5-cm^{-1} resolution to separate the HCl lines from the lines of interference. In Fig. 4a the HCl doublets can be easily discerned when compared to a background spectrum with no HCl present, Fig. 4b. Figure 4a is a portion of a typical spectrum acquired during the 51A launch. This figure shows only the lines within the P branch. The R branch is unusable because of domination by water vapor bands at 2.7 and 3.2 μm. The P(5) line was used to determine the HCl concentrations because it had the least interference.

3.0 APPARATUS

The Shuttle launches took place at KSC Pad 39A. Figure 1 shows the major features of the launch pad and the AEDC equipment location. The test apparatus consisted of an FTS and a collimated light source with associated control and data acquisition instrumentation. The sample path length was 500 m. The distance to the launch structure was approximately 350 m. The equipment was located so that the plume deflected by the flame trench passed through the center of the sample path.

The FTS used was a Block Model RS197 field-rated instrument (Refs. 6 and 7). It was configured to have the maximum sensitivity possible in the spectral region of interest, 3,000 to 2,700 cm^{-1}. This was accomplished by using a germanium beamsplitter on a potassium bromide substrate and an indium antimonide detector cooled to 77 K. The detector dewar had a maximum hold time of 6 hr, so an automatic fill system was developed to replenish the liquid nitrogen (LN$_2$) from a large auxiliary reservoir. The FTS was rigidly mounted to maintain optical alignment with the source during the large vibrations associated with the Shuttle launch. The instrument was enclosed in a Plexiglas® container that was kept at a slight positive pressure with a gaseous nitrogen (N$_2$) purge to reduce the possibility of HCl corrosion (Fig. 5b). The IR radiation entered the FTS through a hole in the Plexiglas container that matched the entrance aperture of the FTS. An O-ring seal was made between the FTS and the container. In this way, the FTS was in the same configuration in the field test as

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in the calibration. The only difference in the optical paths was that the quartz sample cell was fitted with IR transmisive quartz windows on each end.

The source units used in launches 41D and 51A were different. Modifications were made to the equipment for launch 51A because of insight gained during the 41D launch. The original configuration (See Fig. 6a) used in the 41D launch consisted of a Barnes Model 112017 blackbody with collimator and an Optronics Model 100U, 1,000-w tungsten halogen lamp with a 25.4-cm Cassegrain telescope used as a collimator. The use of multiple sources was required to provide adequate intensity since the FTS was located 500 m distant and also as insurance against optical misalignment from the shock of the booster ignition. In the second configuration (See Fig. 6b), for the 51A launch, three, 30.48-cm spherical mirrors with 1,000-w tungsten halogen lamps at their focal points were used to provide an intensity increase of 400 percent. In each case the sources were securely mounted and covered with a hood that provided protection from inclement weather and SRB plume debris. The sources were mounted so that the optical path between the FTS and sources was approximately 1.2 m above the ground (Fig. 6b).

The digital data acquisition system collected a set of 124 interferograms (the raw data) during each sampling period of approximately 2 min. Each set was averaged and stored on magnetic tape as one data point. A spectrum is obtained by taking the Fourier transform of the interferogram (Ref. 6). For launch 41D, data points were collected every 20 min. This time interval was reduced to 10 min for 51A after improvements were made to the software that reduced the processing time from 17 to 8 min. The data were not converted to the spectral domain until later in order to permit the collection of additional data during the postlaunch period.

4.0 CALIBRATION AND ANALYSIS

The absorption technique involved the comparison of spectral data acquired in the field with similar data acquired in the laboratory. As explained in Section 2.0, calibration data generated in the laboratory were used in lieu of published HCl absorption coefficients to negate the influence of the spectrometer instrument line shape.

In the laboratory (Fig. 5a), a previously evacuated quartz sample cell (2.54 diam by 25.4 cm) was filled with mixtures of HCl and dry N_2 with known concentrations simulating the absorption expected following the launch. The concentration of HCl in the sample cell is stated in terms of partial pressures (x) with units of psia, and the concentration (y) in the field is expressed as parts per million (ppm). The relationship is $x/14.7 = y/1,000,000$. Specific sample cell concentrations of HCl were achieved using a partial pressure technique in which

the cell was filled in several stages. Each stage consisted of partially evacuating the cell followed by bringing it back up to 14.7 psia with dry N_2. This process was continued until the desired partial pressure of HCl was reached. To simulate the field conditions, the concentrations used in the laboratory were greater by an amount dictated by Beer's law. A simple form of Beer's law,

$$\ln(I/I_o) = -ABC$$

where

I = transmitted radiation

I_0 = incident radiation

A = absorptivity (constant at a given wavelength)

B = path length

C = concentration of the absorbing medium

states that the ratio of I/I_o will remain constant if C is varied inversely to B. For example, I/I_o is equivalent for a gas at either 1 psia over a 1-m path or for 10 psia over 0.1 m. Therefore, in the laboratory the concentrations needed to be greater by a factor of 1,968 (the ratio of the range in the field, 500 m, to the cell length, 25.4 cm).

A set of nine spectra corresponding to nine calibration pressures were obtained. The x axis of these curves is in terms of path-averaged concentrations over 500 m. Calibration curves were obtained by plotting $\ln(I_o/I)$ versus x for six P lines. The plots are shown in Figs. 7a through f. The partial pressures of HCl, in psia, used in the test cell were 0.018, 0.036, 0.053, 0.080, 0.120, 0.181, 0.272, 0.544, and 1.633. The conversion relationship to the equivalent field concentration is given by y (ppm) = 34.6 x(psia).

The analysis of the KSC spectra consisted of measuring the difference between the baseline and the peak depth of the six P absorption lines. An important feature of this technique is that atmospheric haze does not invalidate the measurement. Atmospheric scattering attributable to haze does not affect the procedure since both I and I_o (Fig. 2b) are influenced by the same amount, leaving the ratio I/I_o constant. This feature negates the necessity of performing an instrument or source calibration.

The error associated with the resultant measurements of the 41D launch is estimated to be ± 19 percent (root sum of the squares). This error is caused by an error of ± 10 percent because of pressure transducer uncertainty, ± 10-percent gas-handling technique, ± 10 percent

in FTS measurement uncertainty, and ±8 percent in data handling (digitization and processing). The error associated with the resultant measurements of the 51A launch is estimated to be ±15 percent (root sum of the squares). This reduction in error is caused by the use of the alternate source unit with a higher intensity during the second measurement. The FTS measurement uncertainty was reduced to ±3 percent, and the data handling uncertainty was reduced to ±2 percent.

5.0 RESULTS

The application of the IR absorption technique following the 41D launch showed the presence of average concentrations of gaseous HCl as great as 4 ppm (±19 percent). Figure 4a is a representative spectrum taken postlaunch. The HCl lines are clearly apparent among other atmospheric absorption lines. Figure 8 gives the concentration of gaseous HCl as yielded by examination of five $H^{35}Cl$ absorption lines. The spread in the results is attributed to the presence of absorption lines of other molecules. Note that in Fig. 8 the concentration determined using the P(5) line is less than concentrations determined using the other lines. In the case of most of the HCl absorption lines, their frequencies are nearly the same as other atmospheric constituents, such as HDO and H_2O (Ref. 5). Therefore, the resultant absorption is greater than that caused only by the HCl. Since it is difficult to determine how much of the absorption is caused by the other molecules, the most isolated line, the P(5) line, was used to determine the HCl concentration.

The concentration peaked approximately 100 min postlaunch, remained high for nearly 1 hr, and then began to diminish. There unfortunately exists a gap in the data because of a period in which instrumentation was realigned following the loss of one of the sources during the high vibration experienced during the launch. The instrumentation was operated for three days following the launch, and HCl was detected only in the 6-hr interval following the launch.

Data obtained from the 51A launch are better in two ways. Data were acquired more frequently and with an improvement in the signal-to-noise ratio by nearly a factor of four. During the 51A launch, higher HCl concentrations were measured than were detected during the 41D launch. Figure 9 is a summary of six concentration curves from the P-branch lines. The curves have a significant scatter caused by absorption attributed to other molecules present in the sample path. The most isolated line again is the P(5) line. Figure 10 shows the best estimate of the HCl concentration. The HCl concentration peaked at about 9 ppm ±15 percent approximately 1 hr postlaunch, fluctuated for about an hour, and then decayed. In the two days following the launch, HCl was detected in minute quantities after sunrise until early afternoon. Long-term, low levels of HCl were visible in the 51A launch either because of

greater revolatilization attributable to atmospheric and ground conditions or better signal-to-noise ratio. Atmospheric conditions during the measurement periods of both launches are available (Refs. 8 and 9).

6.0 SUMMARY

The objectives of the project were completely fulfilled. An unobtrusive absorption technique to monitor concentrations of gaseous hydrogen chloride was developed and then applied on two space shuttle launches at the Kennedy Space Center. The technique developed exploited the intrinsic property of gaseous HCl to absorb IR radiation in specific, narrow, spectral lines. This IR absorption is measured by a Fourier Transform Spectrometer that features accuracy and precision without a calibrated source. The minimum detectable concentration of the instrument is 0.10 ppm with an error of 15 percent (obtained by taking the square root of the sum of the squares of all possible errors or uncertainties in the measurement system including calibration). The application portion of this project enabled refinement of field use of the measurement technique. Increased source radiance and larger source collimating optics improved the signal-to-noise ratio by a factor of four. Improvement in data processing software decreased uncertainty by 4 percent.

Measured quantities of gaseous HCl following launches of both 41D and 51A displayed similar trends. The concentration after each launch first increased, then decreased, then increased to a maximum approximately 100 sec after the launch. The concentration decreased gradually to less than 1 ppm approximately 10 hr after each launch. The peak concentration measured was 4 and 9 ppm for 41D and 51A, respectively. For two days after the 51A launch only, detectable levels were recorded for a period of approximately 6 hr following sunrise. Atmospheric and ground conditions were different for each launch (Refs. 8 and 9). Additional considerations in interpreting the concentration levels are that the data are both path and time averaged, and that the ground scar from the plume makes up approximately 60 percent of the 500-m sample path length. These considerations imply that the concentration along the path is not uniform. Additionally only gaseous HCl will be detected by this technique.

7.0 RECOMMENDATIONS

Improvements to the instrument developed on this project can be made in two areas. The signal can be increased by enlarging the collection optics on the FTS, and the noise can be reduced by increasing the data averaging period. Some improvement in calibration accuracy could be realized by using gas-mixture ratios prepared by the National Bureau of Standards.

The technique developed by this project could use computed tomography with multiple paths to generate a two-dimensional map of HCl concentration levels to determine areas of highest concentration and change over time. This technique would enable determination of safe areas around solid-propellant rocket motor launch complexes where people, wildlife,

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or machinery may be adversely impacted. Additional analysis (not within the scope of this project) should be conducted to determine the impact of atmospheric and ground conditions, aerosol entrapment of HCl, and flame trench cooling water runoff and holding pond contributions to gaseous HCl concentration levels.

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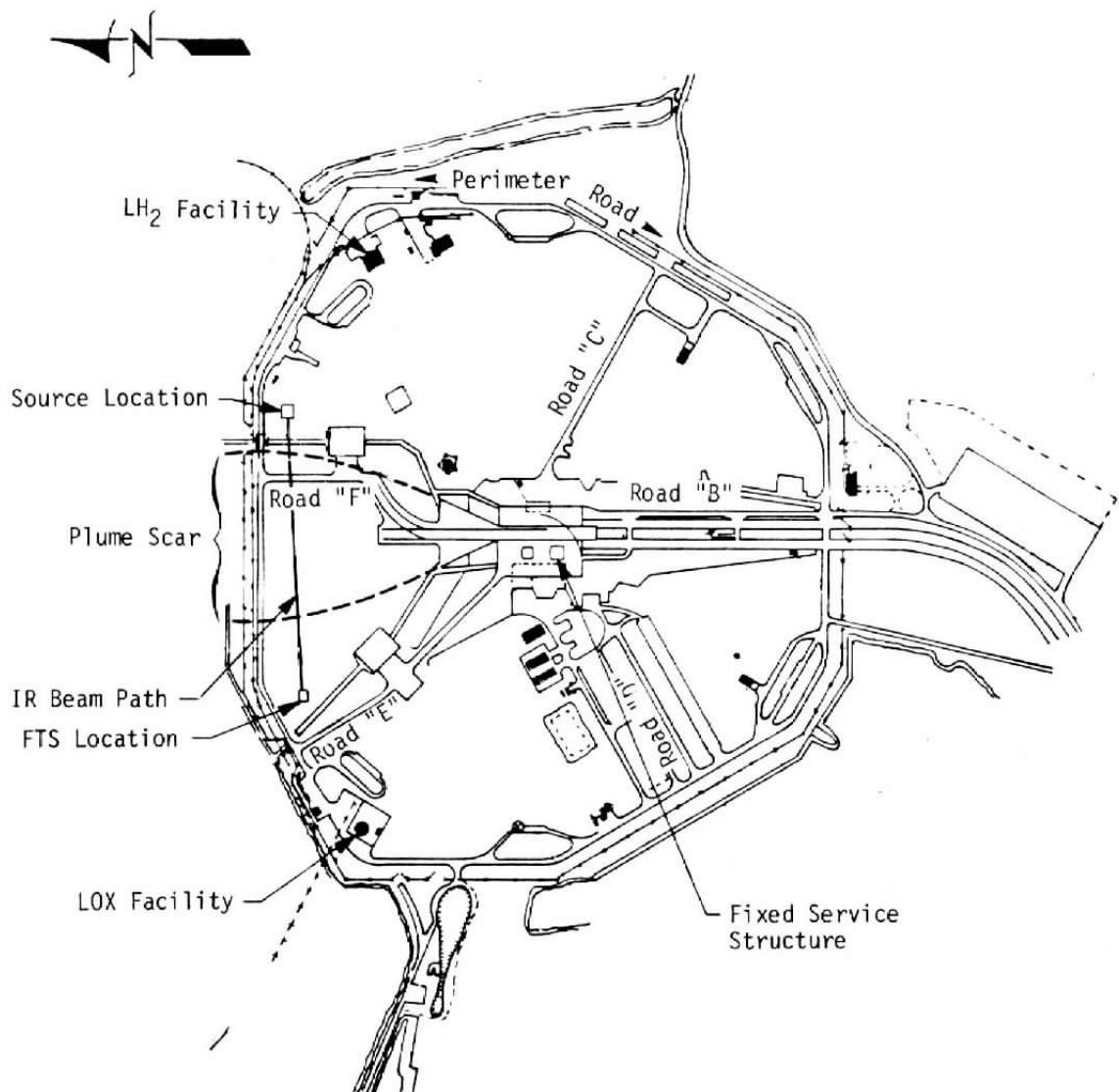
Figure 1. Kennedy Space Center 39A launch pad.
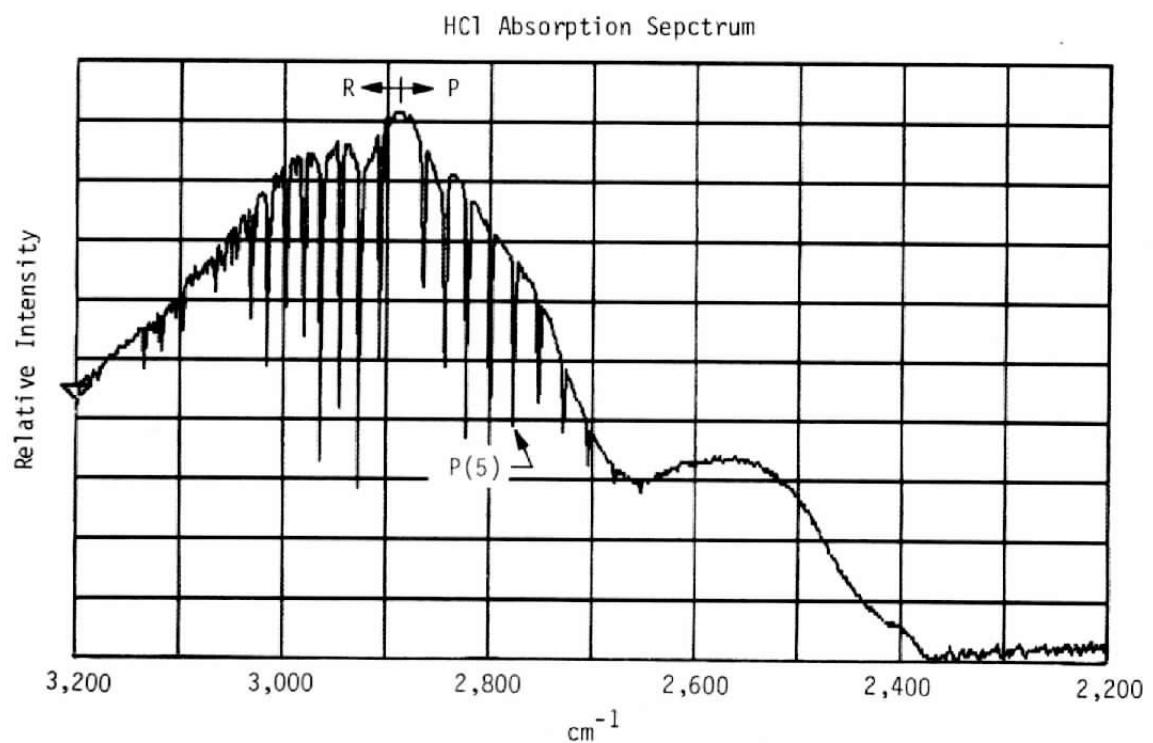
a. Covering 3,200 to 2,200 cm^{-1}
Figure 2. Sample spectrum showing HCl fundamental
absorption band.
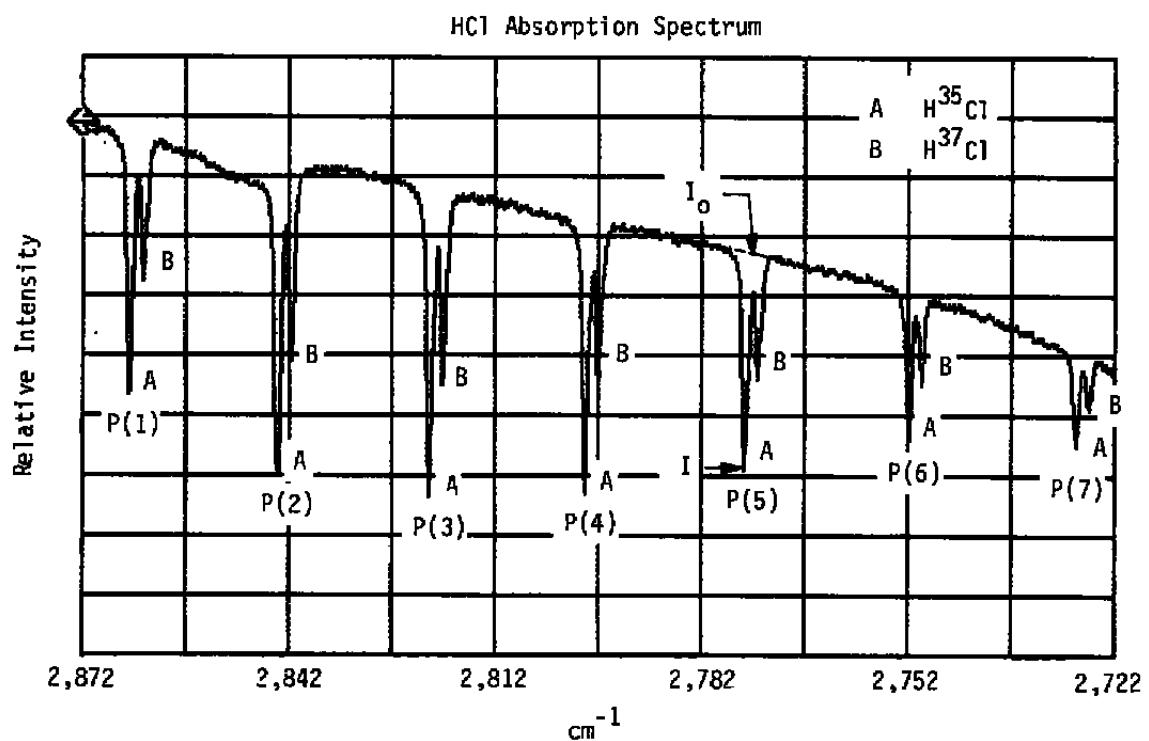
b. Showing only the P branch and how I_0 and I are determined

Figure 2. Concluded.
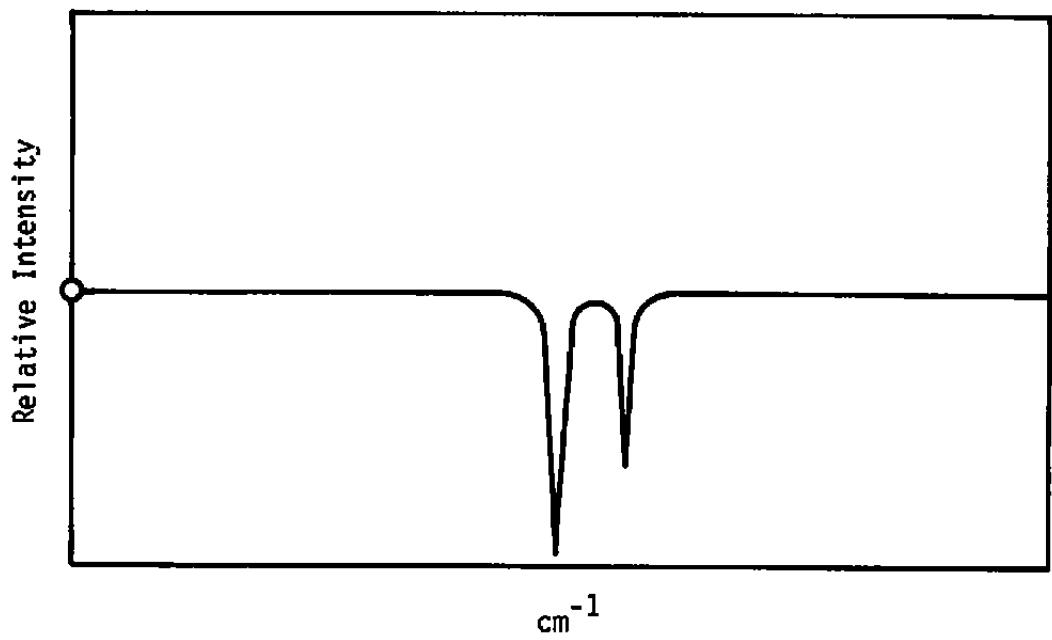
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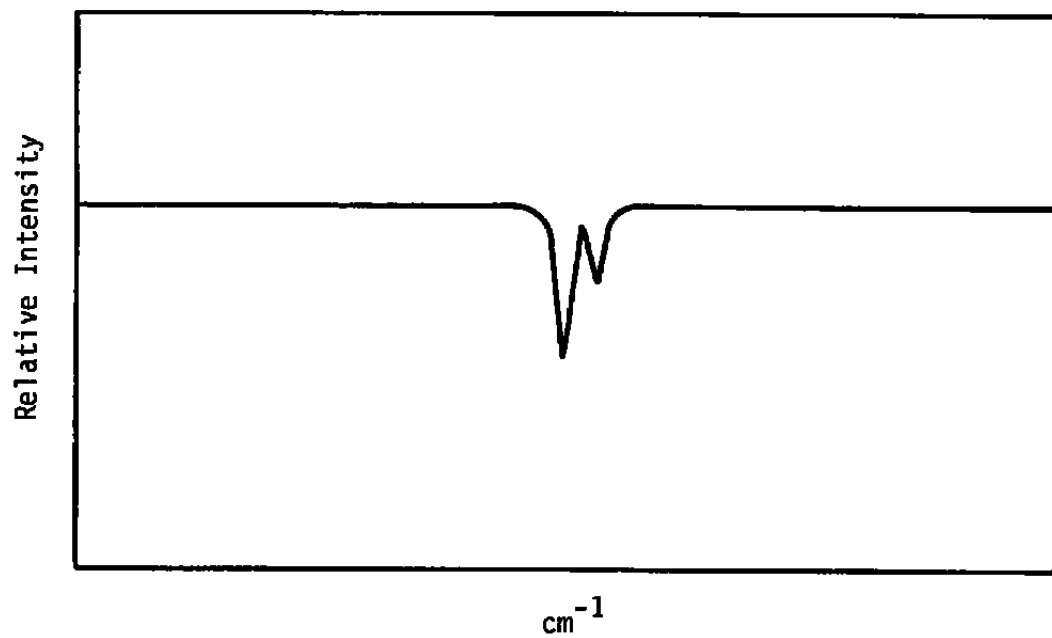

b. Convolved with the ILS
Figure 3. P(1) absorption line.
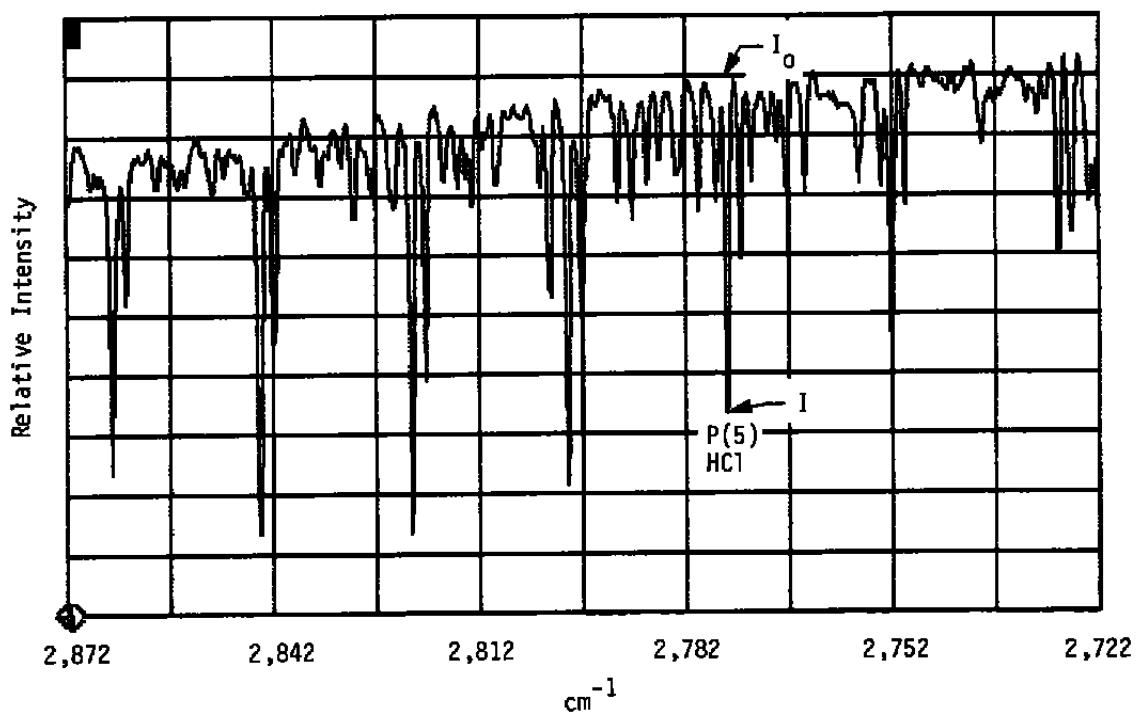
a. Typical spectrum obtained after the 51A launch.
Figure 4. 51A launch spectra.
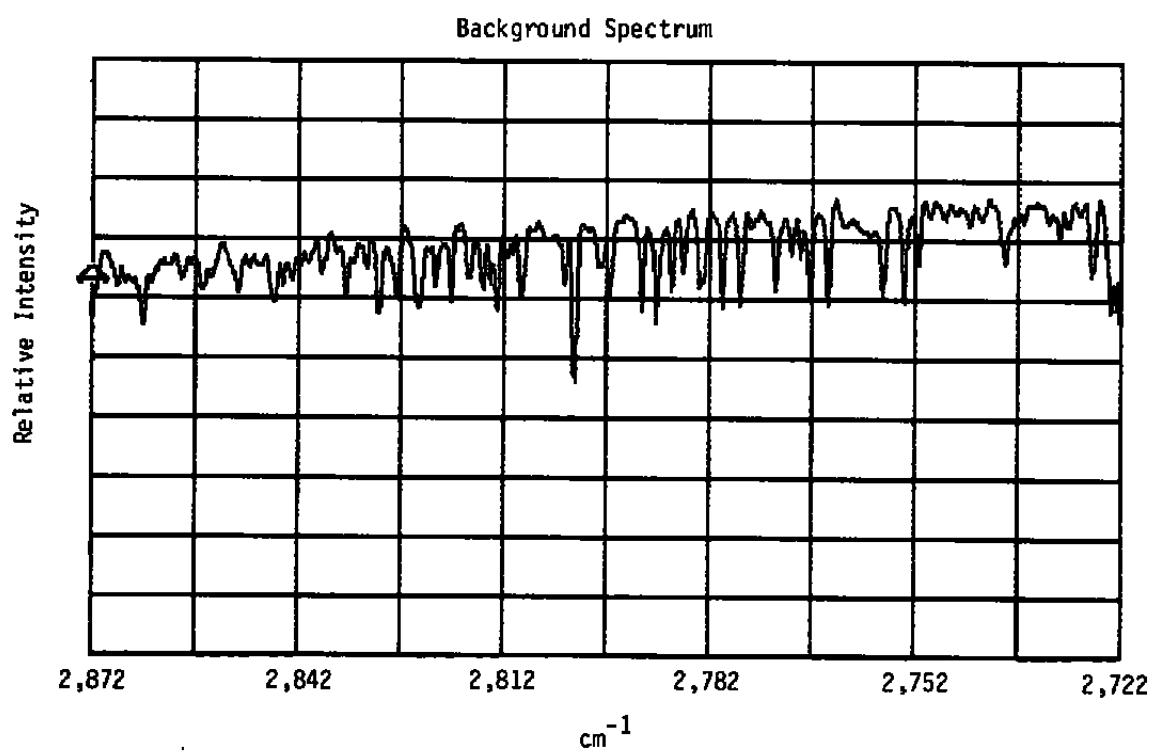
b. Background spectrum obtained before the 51A launch
Figure 4. Concluded.
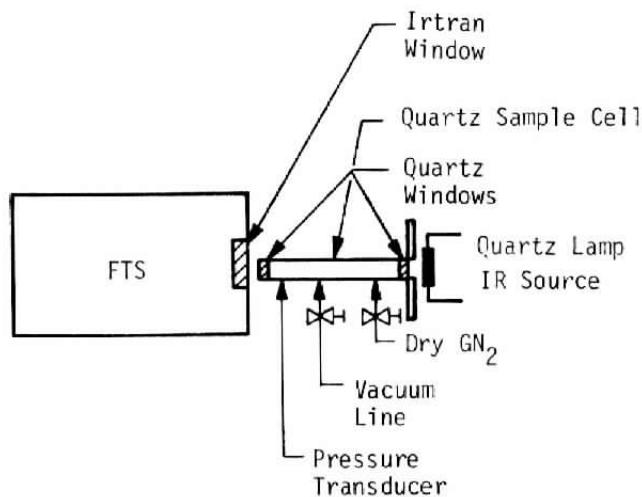
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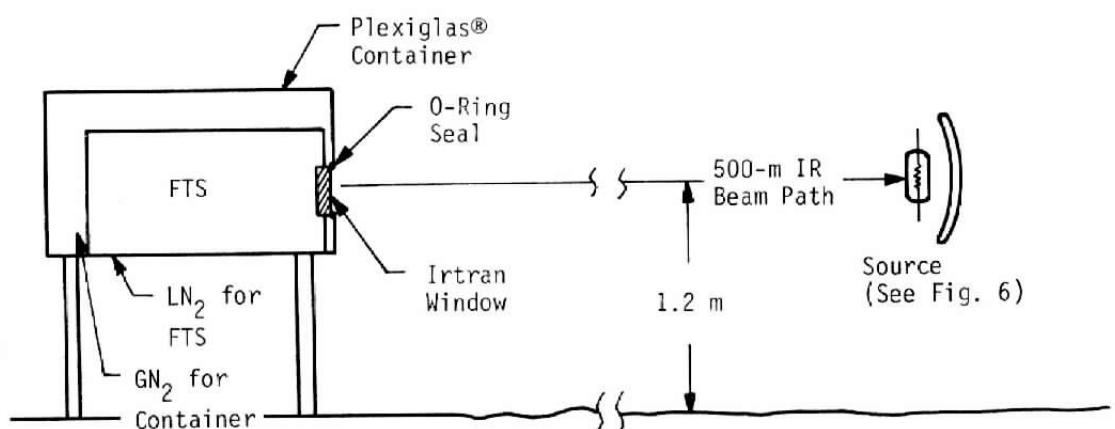
b. Test setup
Figure 5. FTS schematic.
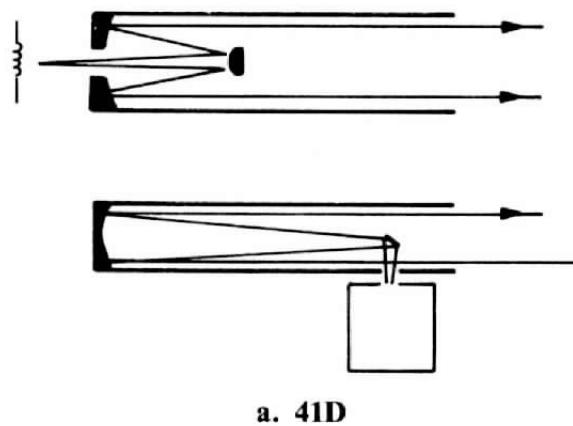
a. 41D
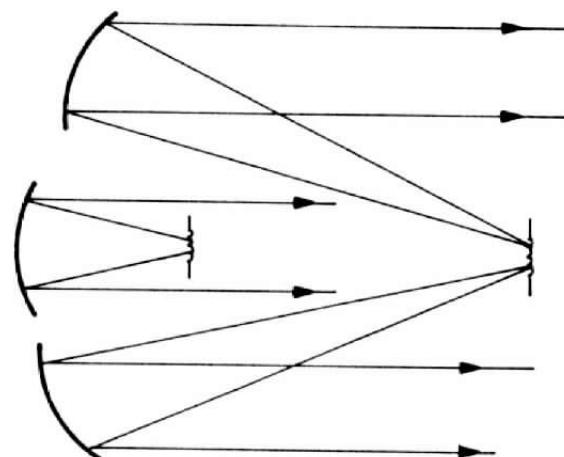
b. 51A
Figure 6. Source configuration.
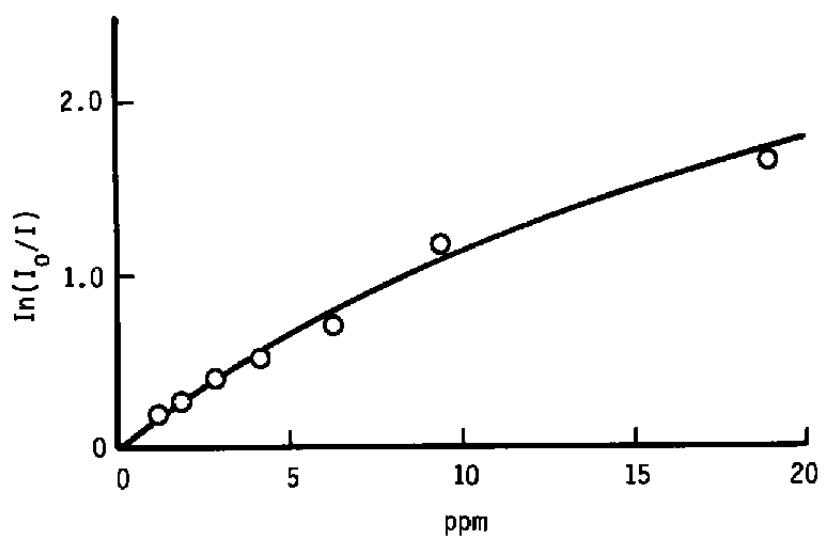
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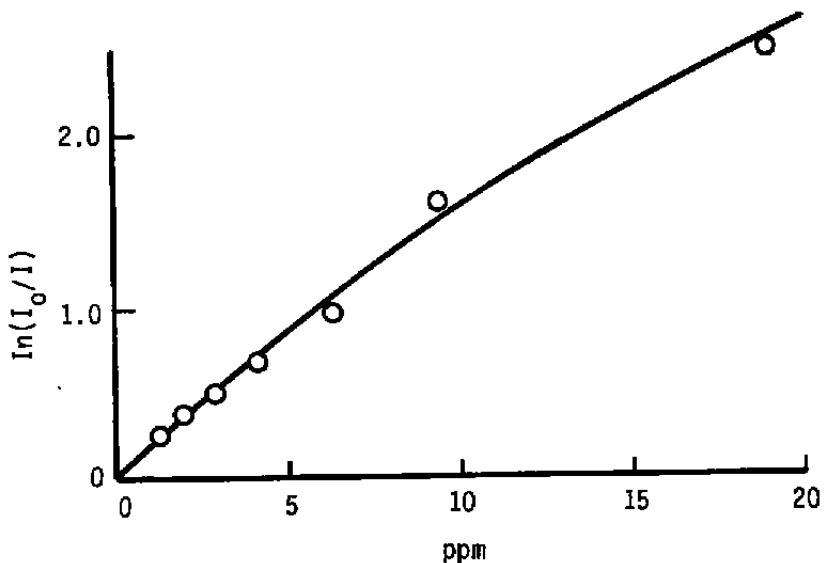

b. P(2) line
Figure 7. Calibration curves for HCl cells.
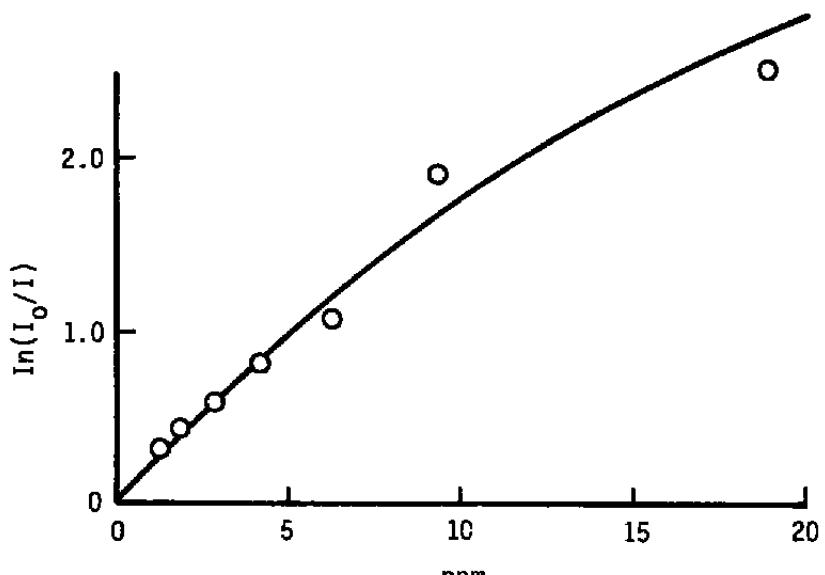
c. P(3) line
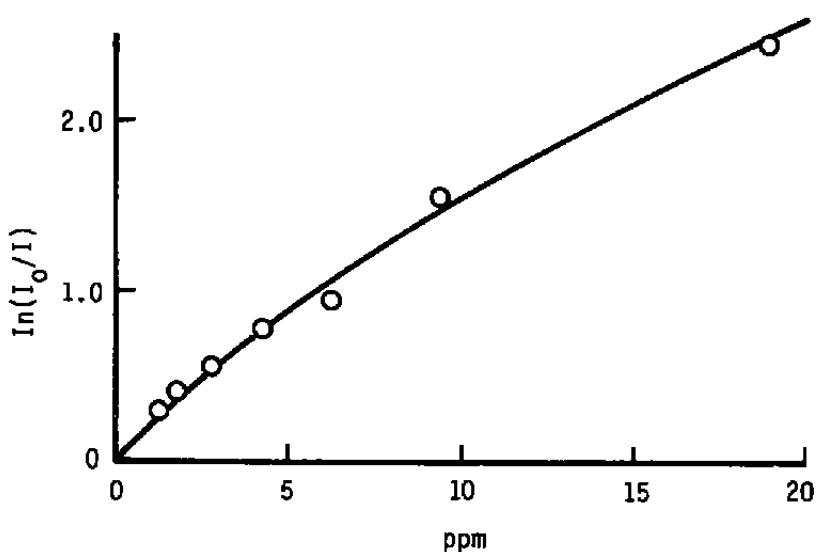
d. P(4) line
Figure 7. Continued.

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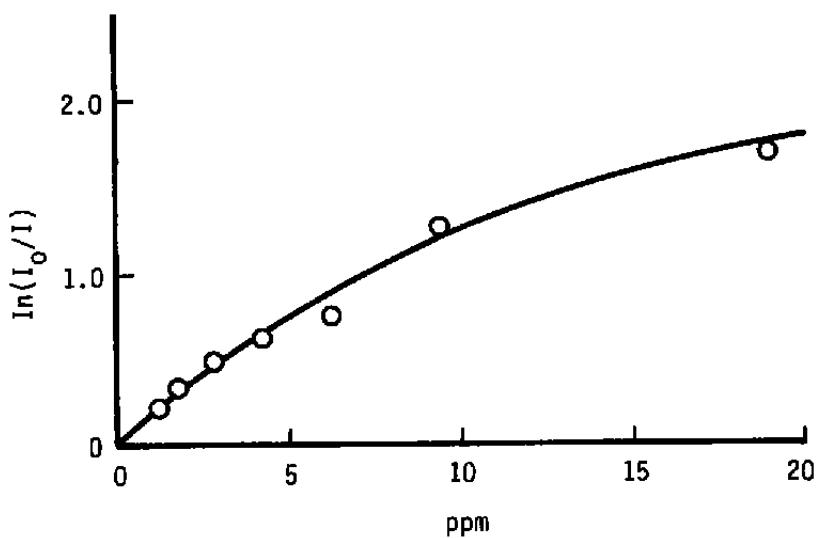
e. P(5) line
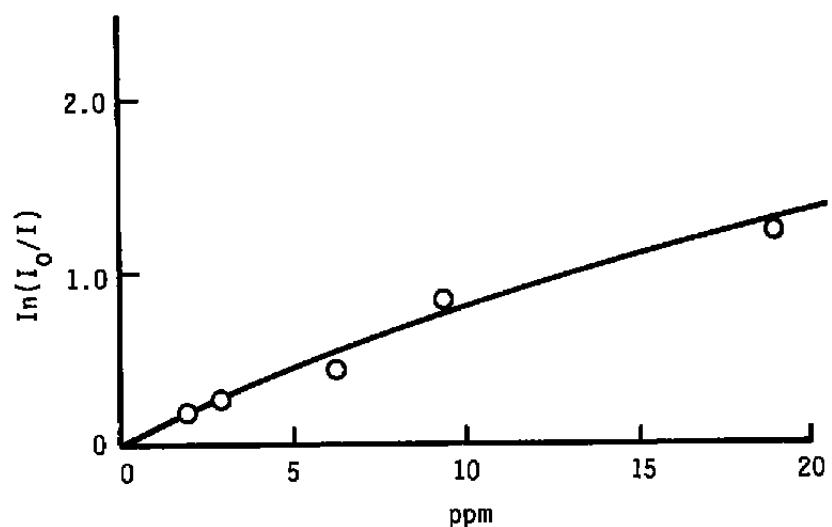
f. P(6) line
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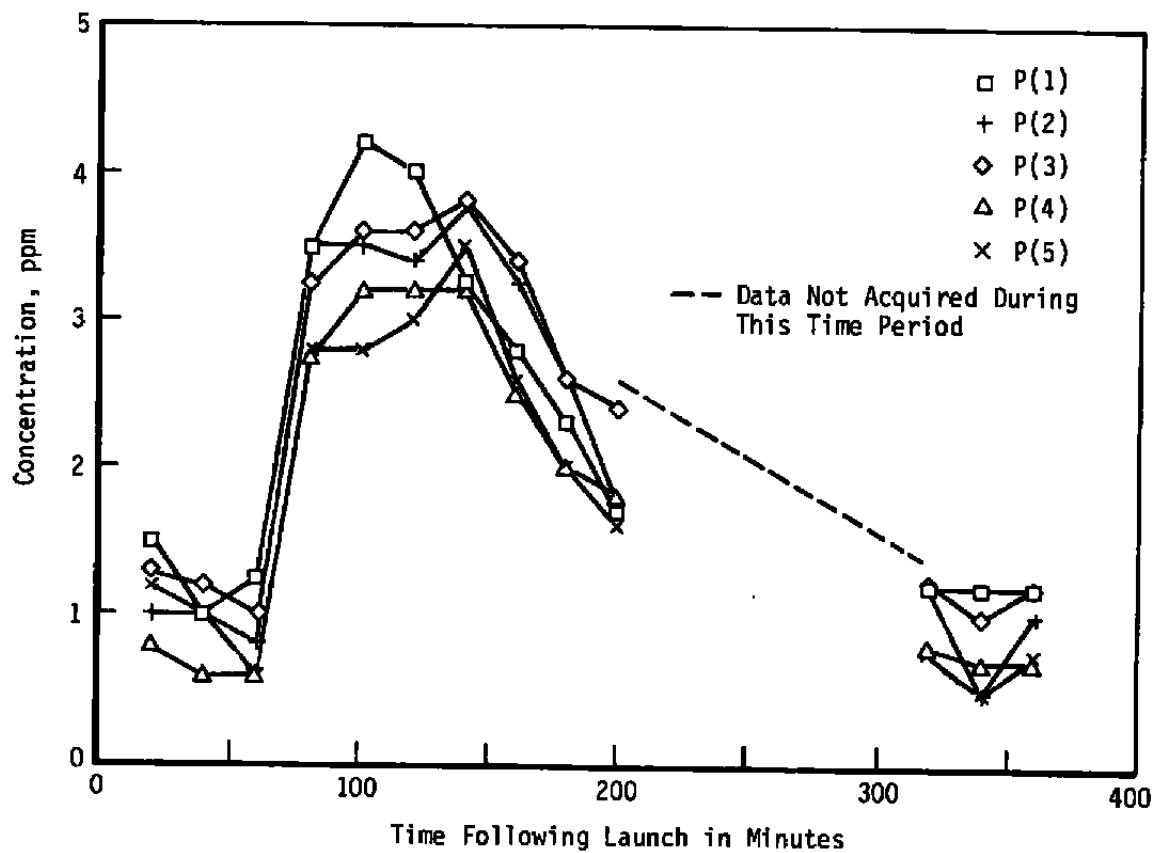
Figure 8. Summary of 41D HCl concentrations measured using several P-branch absorption lines.
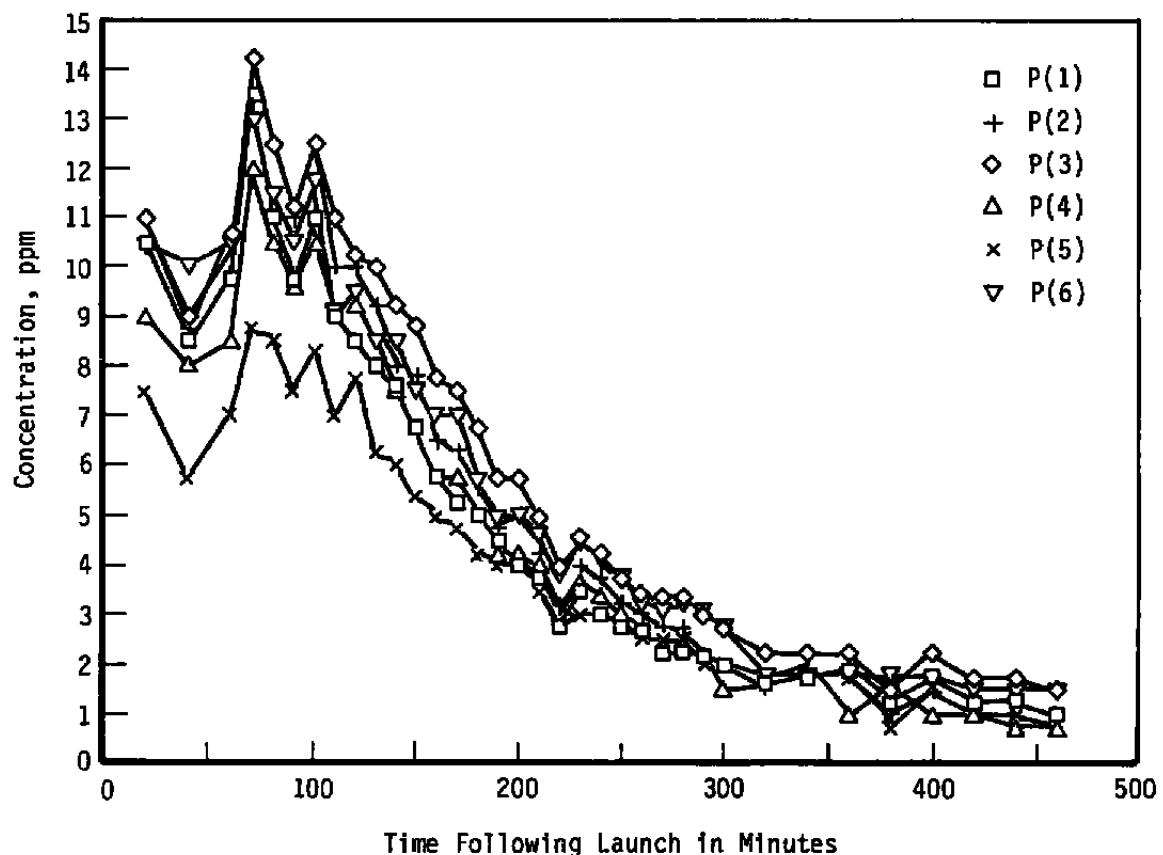
Figure 9. Summary of 51A HCl concentrations measured using several P-branch absorption lines.
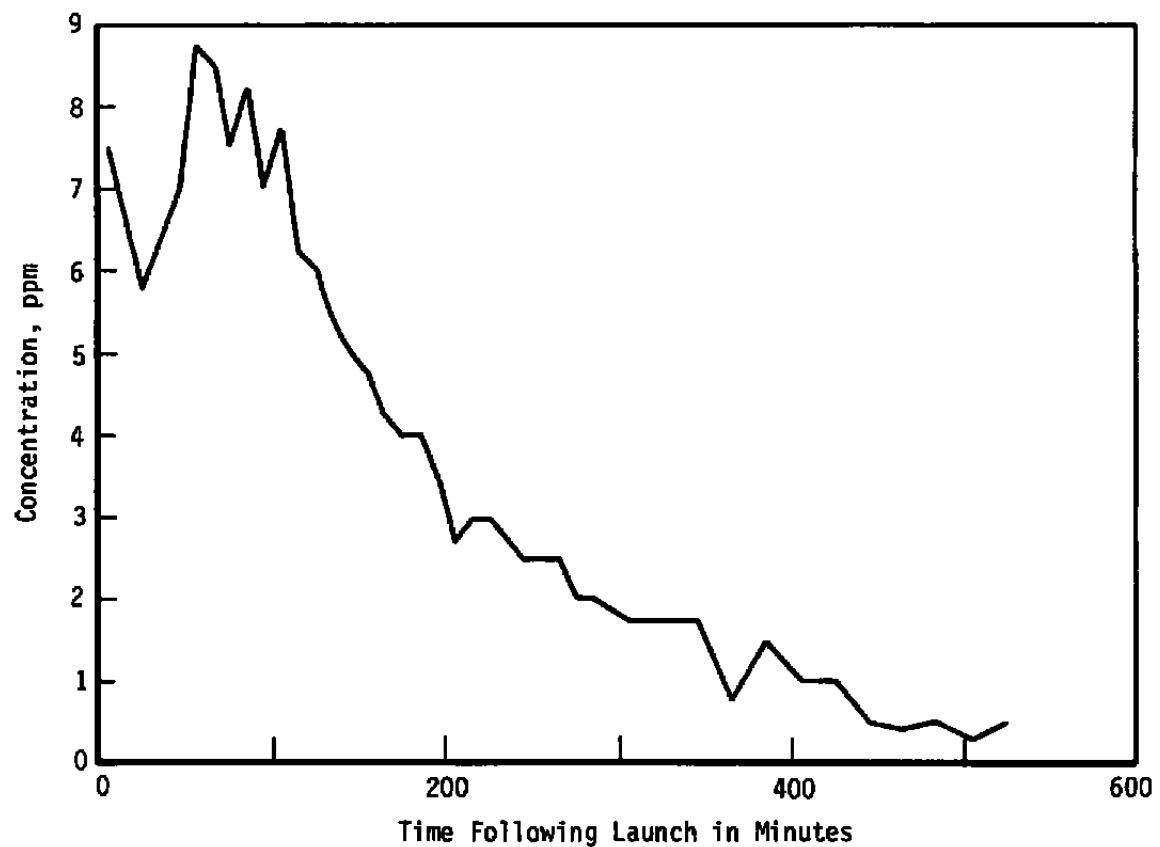
Figure 10. 51A HCl concentration using P(5) line for 10 hr
following launch.